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DICTIONARY FILE UPDATES:  17 OCT 2007  HIGHEST RN 950885-37-7

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http://www.cas.org/support/stngen/stndoc/properties.html

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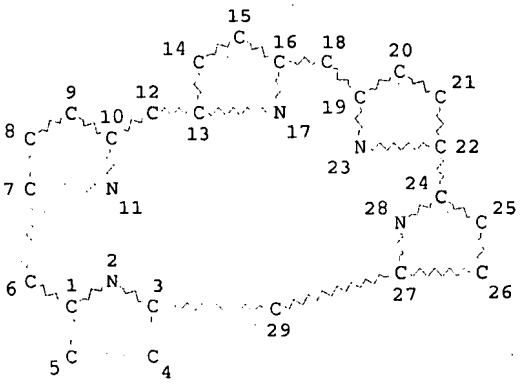

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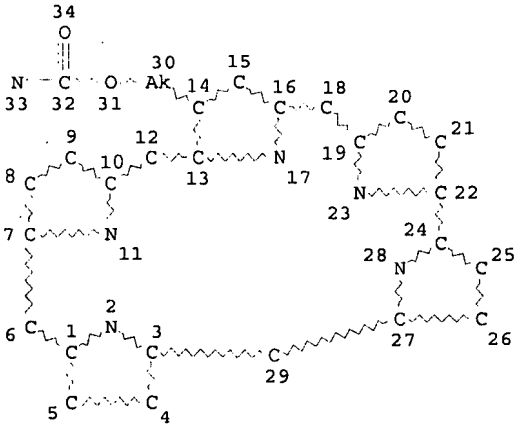

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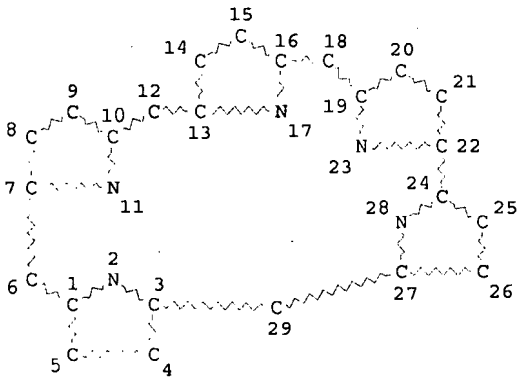

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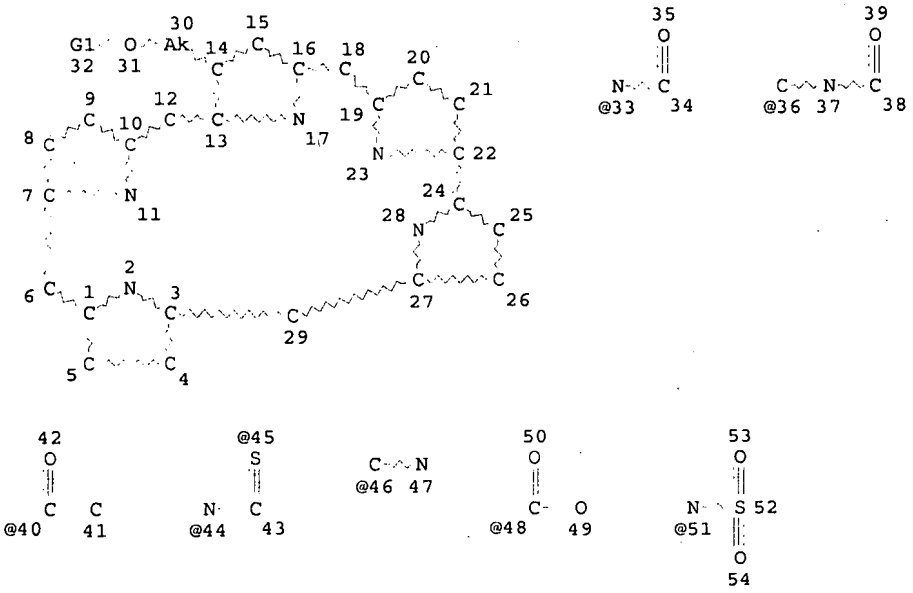

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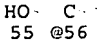

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FILE LAST UPDATED: 17 Oct 2007 (20071017/ED)

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L14 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:162374 HCAPLUS
DN 146:492765
TI Synthesis and biologic properties of hydrophilic sapphyrins, a new class of tumor-selective inhibitors of gene expression
AU Wang, Zhong; Lecane, Philip S.; Thiemann, Patricia; Fan, Qing; Cortez, Cecilia; Ma, Xuan; Tonev, Danielle; Miles, Dale; Naumovski, Louie; Miller, Richard A.; **Magda, Darren**; Cho, Dong-Gyu; Sessler, Jonathan L.; Pike, Brian L.; Yeligar, Samantha M.; Karaman, Mazen W.; Hacia, Joseph G.
CS Pharmacyclics, Inc., Sunnyvale, CA, USA
SO Molecular Cancer (2007), 6, No pp. given
CODEN: MCOACG; ISSN: 1476-4598
URL: http://www.molecular-cancer.com/content/pdf/1476-4598-6-9.pdf
PB BioMed Central Ltd.
DT Journal; (online computer file)
LA English
AB Background: Sapphyrin analogs and related porphyrin-like species have attracted attention as anticancer agents due to their selective localization in various cancers, including hematol. malignancies, relative to surrounding tissues. Sapphyrins are electron affinic compds. that generate high yields of singlet oxygen formation. Although initially explored in the context of photodynamic therapy, sapphyrins have intrinsic anticancer activity that is independent of their photosensitizing properties. However, the mechanisms for their anticancer activity have not been fully elucidated. Results: the authors have prepared a series of hydrophilic sapphyrins and evaluated their effect on proliferation, uptake, and cell death in adherent human lung (A549) and prostate (PC3) cancer cell lines and in an A549 xenograft tumor model. PCI-2050, the sapphyrin derivative with the highest in vitro growth inhibitory activity, significantly lowered 5-bromo-2'-deoxyuridine incorporation in S-phase A549 cells by 60% within eight hours and increased levels of reactive oxygen species within four hours. The growth inhibition pattern of PCI-2050 in the National Cancer Institute 60 cell line screen correlated most closely using the COMPARE algorithm with known transcriptional or translational inhibitors. Gene expression analyses conducted on A549 plateau phase cultures treated with PCI-2050 uncovered wide-spread decreases in mRNA levels, which especially affected short-lived transcripts. Intriguingly, PCI-2050 increased the levels of transcripts involved in RNA processing and trafficking, transcriptional regulation, and chromatin remodeling. The authors propose that these changes reflect the activation of cellular processes aimed at countering the observed wide-spread redns. in transcript levels. In the authors' A549 xenograft model, the two lead compds., PCI-2050 and PCI-2022, showed similar tumor distributions despite differences in plasma and kidney level profiles. This provides a possible explanation for the better tolerance of PCI-2022 relative to PCI-2050. Conclusion: Hydrophilic sapphyrins were found to display promise as novel agents that localize to tumors, generate oxidative stress, and inhibit gene expression.
IT **924905-80-6**, PCI 2050 **936576-25-9**, PCI 2012
936576-26-0, PCI 2022 **936576-27-1**, PCI 2042
RL: ADV (Adverse effect, including toxicity); DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(hydrophilic sapphyrins were found to display promise as novel agents that localize to tumors, generate oxidative stress, and inhibit gene expression)
RN 924905-80-6 HCAPLUS
CN 5,8,11-Trioxa-2-azadodecanoic acid, 2-[2-[2-(2-methoxyethoxy)ethoxy]ethyl]-, 1,1'-[(4,13,14,23-tetraethyl-3,8,19,24-tetramethyl-25,26,27,28,29-pentaazahexacyclo[20.2.1.12,5.17,10.112,15.117,20]nonacosa-1,3,5,7(28),8,10,12,14,16,18,20(26),21,23-tridecaene-9,18-diyl)di-3,1-propanediyl] ester (CA INDEX NAME)

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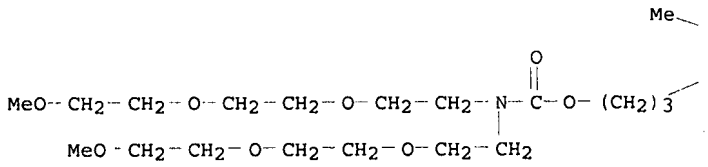

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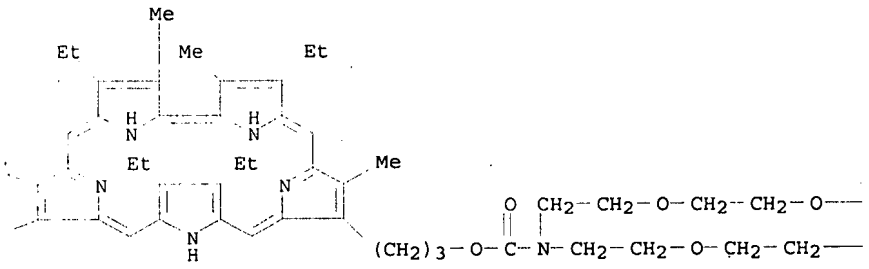

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RN 936576-25-9 HCAPLUS
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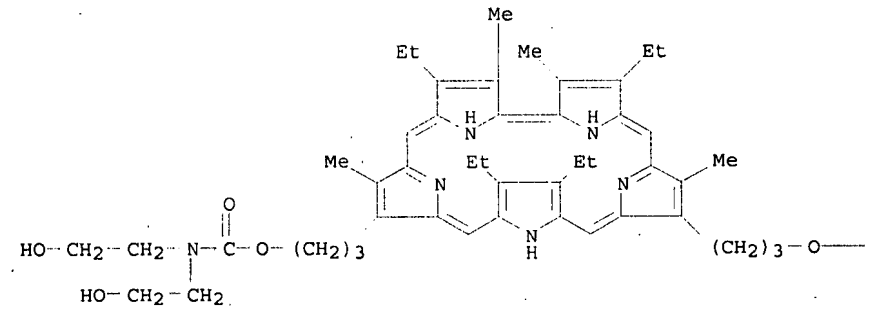

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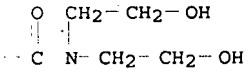

RN 936576-26-0 HCAPLUS
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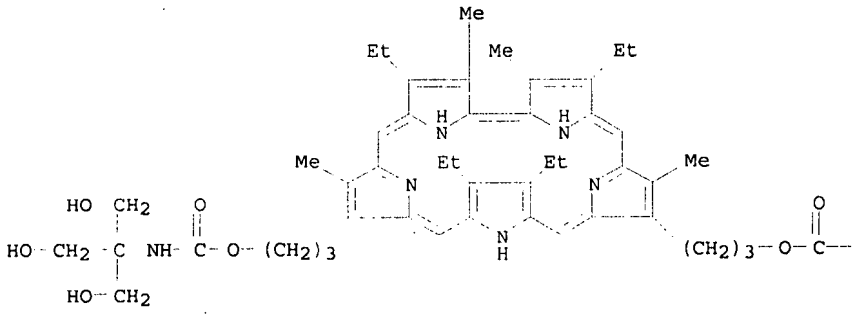

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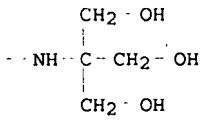

RN 936576-27-1 HCAPLUS
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Absolute stereochemistry.

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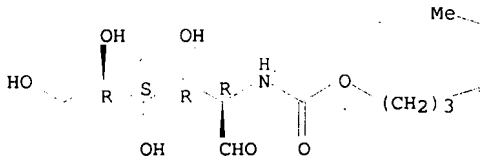

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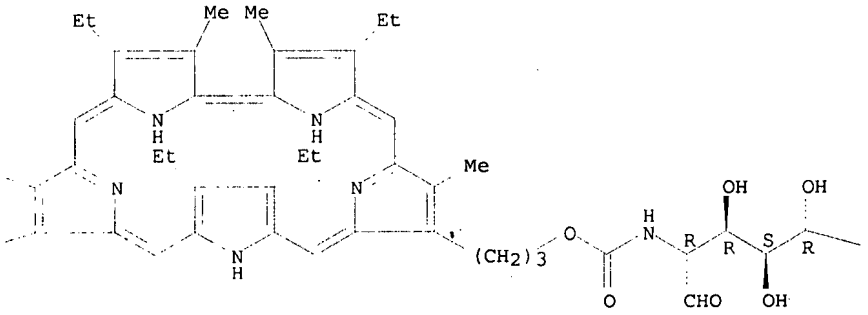

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ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1236185 HCAPLUS
DN 146:220114
TI Tumor localization and antitumor efficacy of novel sapphyrin compounds
AU Naumovski, Louie; Sirisawad, Mint; Lecane, Philip; Chen, Jun; Ramos, Jason; Wang, Zhong; Cortez, Cecilia; **Magda, Darren**; Thiemann, Patti; Boswell, Garry; Miles, Dale; Cho, Dong Gyu; Sessler, Jonathan L.; Miller, Richard
CS Pharmacyclics, Inc., Sunnyvale, CA, USA
SO Molecular Cancer Therapeutics (2006), 5(11), 2798-2805
CODEN: MCTOCF; ISSN: 1535-7163
PB American Association for Cancer Research
DT Journal
LA English
AB Sapphyrins are pentapyrrolic metal-free expanded porphyrins with potential medical use as anticancer agents. The novel sapphyrin derivative, PCI-2050, functionalized with 2-[2-(2-methoxyethoxy)ethoxy]ethoxy groups to enhance

solubility and a modified bipyrrole moiety was more potent in inducing apoptosis than the previously described sapphyrin PCI-2000. Because some sapphyrins may localize to tumors, we took advantage of the intrinsic fluorescence of these compds. to develop a flow cytometry-based assay to track sapphyrin biodistribution in tumor-bearing mice. Ex vivo anal. of sapphyrin-injected animals revealed that PCI-2050 preferentially localized to tumor, whereas PCI-2000 distributed into normal tissues rather than tumor. PCI-2050 uptake in xenograft tumor cells and resultant tumor cell cytotoxicity was dose dependent. To investigate structure-activity relationships, we focused on PCI-2050 and three derivs. that differ by their alkyl substituents on the bipyrrole moiety: PCI-2051, PCI-2052, and PCI-2053. Treatment of Ramos cells in culture or treatment of Ramos xenograft-bearing animals with each of the sapphyrins followed by ex vivo growth of tumor cells revealed the same pattern of cytotoxicity: PCI-2050 > PCI-2052 > PCI-2051 > PCI-2053. Thus, subtle changes in the alkyl substituents on the bipyrrole moiety result in significant changes in antitumor activity. PCI-2050 displayed significant antitumor efficacy in both Ramos and RKO xenograft models without hematol., hepatic, or renal abnormalities as assessed by complete blood counts and serum chemistries. On the basis of these findings, it is concluded that the sapphyrin PCI-2050 warrants further evaluation as a potential anticancer agent due to its intrinsic proapoptotic activity and tumor localization ability.

IT **924905-80-6**, PCI 2050 **924905-81-7**, PCI 2051
924905-82-8, PCI 2052 **924905-83-9**, PCI 2053
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tumor localization and antitumor efficacy of novel sapphyrin compds.)

RN 924905-80-6 HCAPLUS

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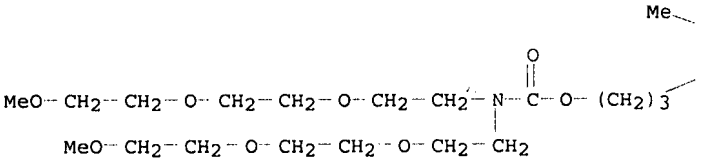

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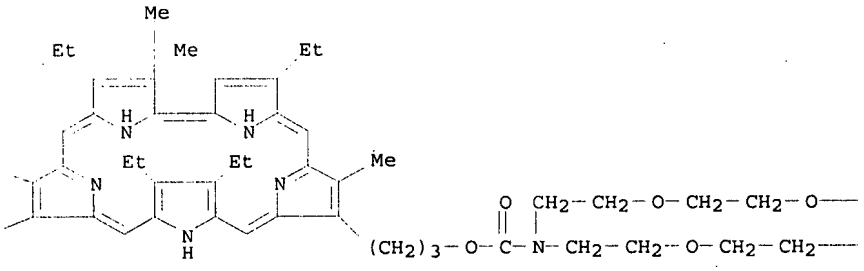

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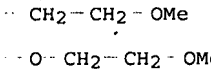

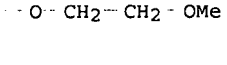

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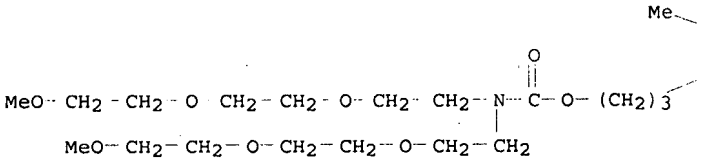

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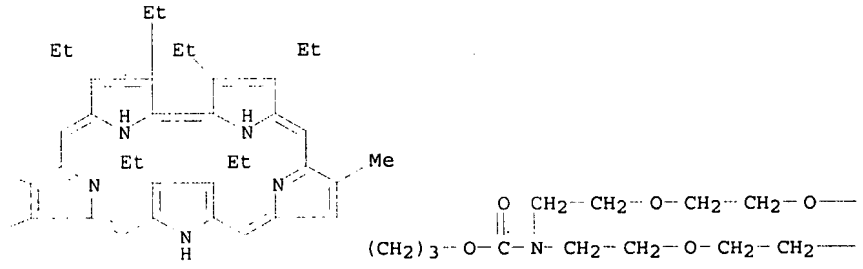

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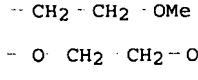

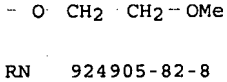

RN 924905-82-8 HCAPLUS

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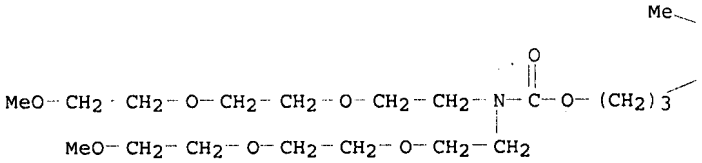

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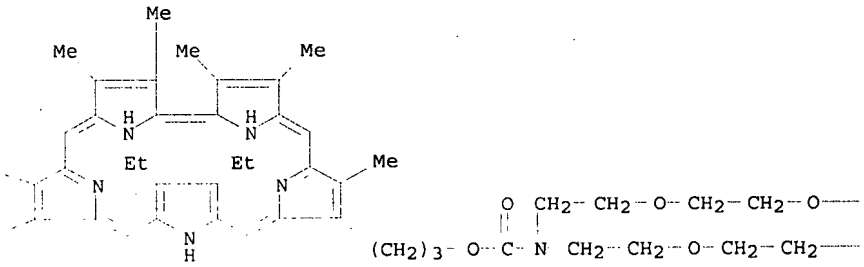

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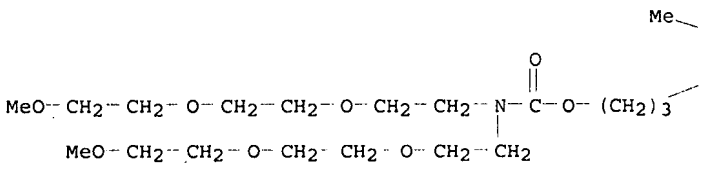

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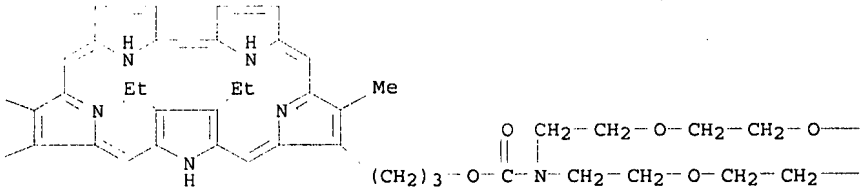

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RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:511839 HCAPLUS
DN 143:259655
TI Sapphyrins induce apoptosis in hematopoietic tumor-derived cell lines and show in vivo antitumor activity
AU Naumovski, Louie; Ramos, Jason; Sirisawad, Mint; Chen, Jun; Thiemann, Patti; Lecane, Philip; **Magda, Darren**; Wang, Zhong; Cortez, Cecilia; Boswell, Garry; Cho, Dong Gyu; Sessler, Jonathan; Miller, Richard
CS Pharmacyclics, Inc., Sunnyvale, CA, 94085, USA
SO Molecular Cancer Therapeutics (2005), 4(6), 968-976
CODEN: MCTOCF; ISSN: 1535-7163
PB American Association for Cancer Research
DT Journal
LA English
AB Sapphyrins are pentapyrrolic, metal-free, expanded porphyrins. In the present study, the activity of sapphyrins as anticancer agents in hematopoietic-derived tumor cells was explored. It was found that a dihydroxylated water-soluble sapphyrin derivative (PCI-2000) is a potent inducer of apoptosis in a wide variety of tumor cell lines including lymphoma (Ramos, DHL-4, and HF-1), leukemia (Jurkat and HL-60), and myeloma (8226/S, 1-310, C2E3, and 1-414). PCI-2000 triggers an apoptotic pathway in these tumor cells as shown by release of cytochrome c from mitochondria; activation of caspases 9, 8, and 3; cleavage of the caspase substrate poly(ADP-ribose) polymerase; and Annexin V binding. Apoptosis can be partially inhibited by overexpression of the antiapoptotic protein Bcl-2 or treatment with benzyloxycarbonyl-valine-alanine-aspartic acid-fluoromethylketone, a cell-permeable caspase inhibitor. Both PCI-2000 and PCI-2010, a tetrahydroxy bis-carbamate derivative of PCI-2000, result in increased levels of phosphorylated p38 mitogen-activated protein kinase. Inhibition of p38 mitogen-activated protein kinase

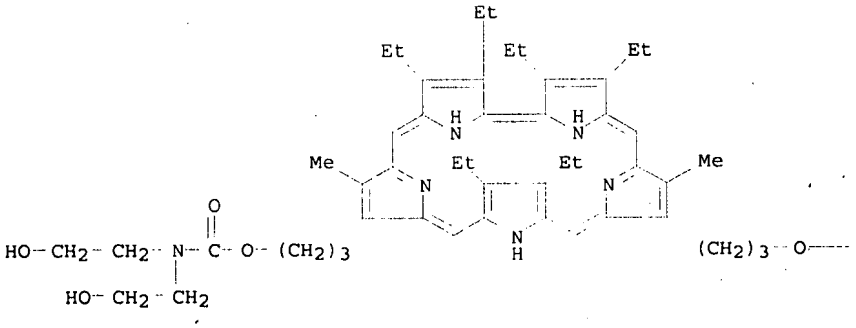
phosphorylation resulted in a synergistic increase of PCI-2000 cytotoxicity. PCI-2010 showed less toxicity in mice than PCI-2000 and was active in slowing the growth of Ramos and HL-60 tumor xenografts in nude mice. These results provide preclin. rationale for the further study of sapphyrins for potential use in the treatment of hematopoietic-derived tumors.

IT **777931-97-2**, PCI 2010
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(sapphyrins induce apoptosis in hematopoietic tumor-derived cell lines and show antitumor activity)

RN 777931-97-2 HCAPLUS

CN Carbamic acid, bis(2-hydroxyethyl)-, (3,4,13,14,23,24-hexaethyl-8,19-dimethyl-25,26,27,28,29-pentaazahexacyclo[20.2.1.12,5.17,10.112,15.117,20]nonacosa-1,3,5,7(28),8,10,12,14,16,18,20(26),21,23-tridecaene-9,18-diyl)di-3,1-propanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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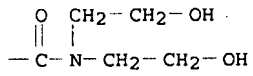

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:872660 HCAPLUS
DN 141:360663
TI Sapphyrins and their uses to treat neoplasm
IN **Magda, Darren**; Sessler, Jonathan L.; Wang, Zhong
PA Pharmacyclics, Inc., USA; Board of Regents, University of Texas System
SO PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2004089300	A2	20041021	2004WO-US10481	20040405
	WO2004089300	A3	20050811		

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AU2004228050	A1	20041021	2004AU-0228050	20040405
CA---2520452	A1	20041021	2004CA-2520452	20040405
EP---1615552	A2	20060118	2004EP-0758893	20040405
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US2006241166	A1	20061026	2006US-0552696	20060713 <--
PRAI 2003US-460846P	P	20030404		
2003US-520275P	P	20031113		
2003US-527510P	P	20031205		
2004WO-US10481	W	20040405		

OS MARPAT 141:360663

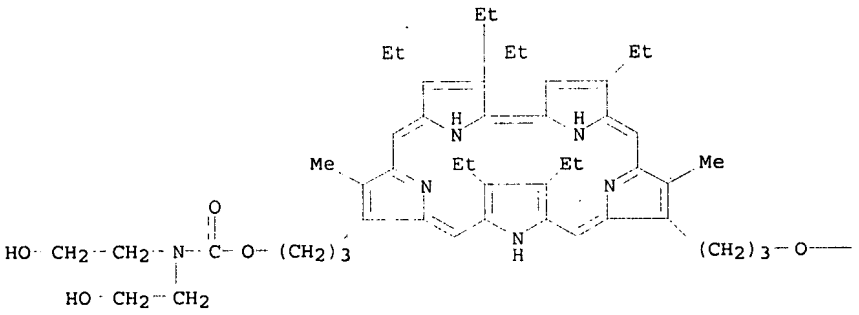
AB The present invention relates to sapphyrins, their pharmaceutical composition, and their utility in treating neoplasm. For example, carbamate-linked tetrahydroxy-sapphyrin was prepared Bishydroxypropyl-sapphyrin (100 mg, 0.145 mmol) and 186 mg (0.725 mmol) of N,N'-disuccinimidyl carbonate were placed in a Schlenk tube, and 187 mg (1.45 mmol) of diisopropylethylamine and 5 mL CH2Cl2 were added, and the reaction mixture was stirred at room temperature for 4 h. Diethanolamine (152 mg, 1.45 mmol) dissolved in 1 mL CH2Cl2 was added, and the resulting mixture was stirred for another hour. The reaction mixture was concentrated to give an oily residue, and purified to yield 75 mg (51%) of tetrahydroxy-carbamate-sapphyrin (as monoacetate). Also, the effects of various sapphyrins when added to Ramos cells in causing cell death were presented.

IT **777931-97-2P 777931-98-3P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of sapphyrins for treatment of neoplasm)

RN 777931-97-2 HCAPLUS

CN Carbamic acid, bis(2-hydroxyethyl)-, (3,4,13,14,23,24-hexaethyl-8,19-dimethyl-25,26,27,28,29-pentaazahexacyclo[20.2.1.12,5.17,10.112,15.117,20]nonacosa-1,3,5,7(28),8,10,12,14,16,18,20(26),21,23-tridecaene-9,18-diyl)di-3,1-propanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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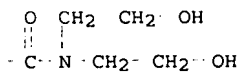

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CN Carbamic acid, bis(2-hydroxyethyl)-, (3,4,13,14,23,24-hexaethyl-8,19-dimethyl-25,26,27,28,29-pentaazahexacyclo[20.2.1.12,5.17,10.112,15.117,20]nonacosa-1,3,5,7(28),8,10,12,14,16,18,20(26),21,23-tridecaene-9,18-diyl)di-3,1-propanediyl ester, monoacetate (salt) (9CI) (CA INDEX NAME)

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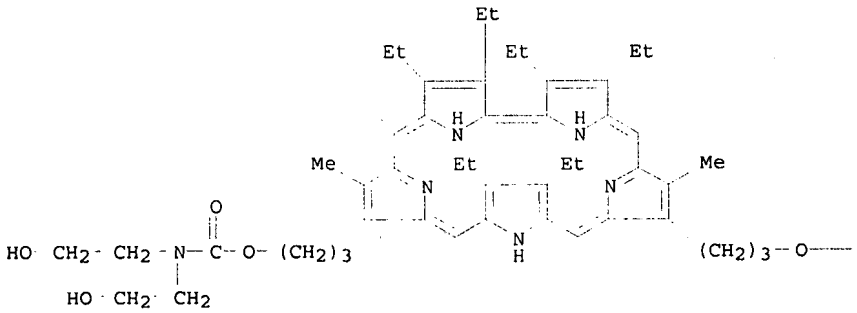
CRN 777931-97-2
CMF C54 H75 N7 O8

PAGE 1-A



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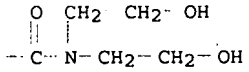
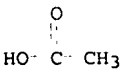


CM 2

CRN 64-19-7
CMF C2 H4 O2



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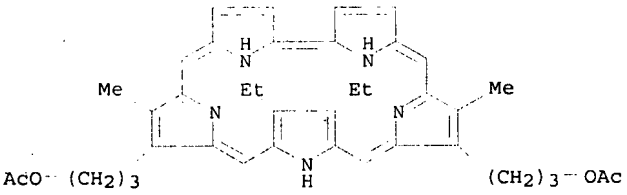
L20 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:314979 HCAPLUS
DN 145:7911
TI Synthesis and Diels-Alder reaction of a sapphyrin derivative
AU Tome, Joao P. C.; Cho, Dong-Gyu; Sessler, Jonathan L.; Neves, Maria G. P. M. S.; Tome, Augusto C.; Silva, Artur M. S.; Cavaleiro, Jose A. S.
CS Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 78712-0165, USA
SO Tetrahedron Letters (2006), 47(18), 3131-3134
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier B.V.
DT Journal
LA English

OS CASREACT 145:7911
AB Sapphyrins participate in Diels-Alder reactions with pentacene affording novel barrelene-fused sapphyrins. The new compds. were synthesized using traditional heating and microwave irradiation conditions. The expts. carried out under microwave irradiation proved cleaner, affording only the monoadduct and in higher yields.
IT **888028-62-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and Diels-Alder reaction of a sapphyrin derivative)
RN 888028-62-4 HCAPLUS
CN 25,26,27,28,29-Pentaazahexacyclo[20.2.1.12,5.17,10.112,15.117,20]nonacosa-1,3,5,7(28),8,10,12,14,16,18,20(26),21,23-tridecaene-9,18-dipropanol, 13,14-diethyl-8,19-dimethyl-, diacetate (ester) (9CI) (CA INDEX NAME)



RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L9 2 L6 AND L8

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L12 73 E3,E6-7
L13 4 L10 AND L12
L14 4 L11,L13

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